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On Prognosis of Growth of Epitaxial Layers during Pulsed Laser Deposition under the Influence of Changes of Parameters

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ABSTRACT: Pulsed laser deposition is one of the most promising modern approaches for producing epitaxial layers. The approach gives a possibility to apply materials with special properties (metals, carbides, etc.) to the surface of parts, which allows restoring geometry, increasing surface strength and corrosion resistance, etc. This paper considers an analytical approach for solution of partial differential equations. This approach has been used for analysis of mass and heat transfer in reaction chamber during growth of the epitaxial layers by using pulse laser deposition. Changing of mass and heat transfer is investigated depending on a number of parameters. We consider an analytical approach for analysis of mass and heat transfer. The approach gives a possibility to take into account changing of parameters of processes both in space and time, as well as the nonlinearity of the processes. The approach was used for the analysis of mass and heat transfer in the reaction chamber during growth of epitaxial layer by using pulsed laser deposition. Changing of mass and heat transfer was investigated depending on series of parameters. The approach for analysis mass and heat transfer, which were considered in this work, makes it possible to carry out a more adequate prognosis of growth of an epitaxial layer by using pulsed laser deposition in comparison with similar approaches.

KEYWORDS: growth of films; pulsed laser deposition; analytical approach for modeling.

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INTRODUCTION

One of the most promising methods of growing of epitaxial layers is a method based on pulsed laser deposition. This method gives a possibility to grow layers of materials with special properties on the surface of details. The application gives a possibility to restore geometry, increase surface strength and corrosion resistance, to manufacture structures with the required properties [1-10]. In this paper, we consider mass and heat transfer in a reaction chamber during growth of an epitaxial layer by pulsed laser deposition. We introduced an analytical approach for predicting of the considerate process. The approach gives a possibility to take into account nonlinearity of the considerate processes as well as changes of parameters of the process in space and time.

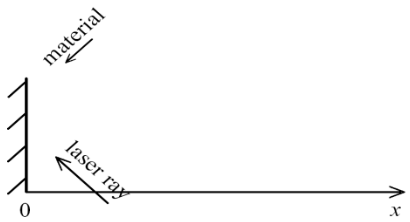

Fig. 1 The direction of motion of the material vaporized during laser deposition

$$c_p\rho\left[\frac{\partial T(x,t)}{\partial t}-u(t)\frac{\partial T(x,t)}{\partial x}\right]=\frac{\partial}{\partial x}\left[\lambda(T)\frac{\partial T(x,t)}{\partial x}\right]+p(x,t), \quad (1)$$

where ρ is the density of the evaporated material; c_p is the specific heat at constant pressure; $T(x,t)$ is the temperature distribution; $\lambda(T)$ is the thermal conductivity (dependence of thermal conductivity on temperature could be approximated by the following relation: $\lambda(T)=\lambda_{ass}\{1+\mu\ [T_d/T(x,t)]^{\varphi}\}$, see, for example, [11]); $p(x,t)$ is the power density of laser radiation; x and t are the current coordinate and time; $\alpha(T)=\lambda(T)/c(T)$ is the thermal diffusivity. Speed of movement of the evaporation boundary is determined by flows J_i of particles evaporated from the surface: $u(t)=\sum_i J_i/\rho_i$, where i means the material used during growth. Boundary and initial conditions could be written in the following form

$$\lambda\left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0}=Q_p\cdot u(t),\ T(\infty,t)=T_r,\ T(x,0)=T_r. \quad (1a)$$

Here T_r is the equilibrium temperature equals

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room temperature; Q_p is the heat of vaporization. We describe the transfer of the growth components using the second Fick law in the following form

$$\frac{\partial C(x,t)}{\partial t} - u(t)\frac{\partial C(x,t)}{\partial x} = \frac{\partial}{\partial x}\left[D_C \frac{\partial C(x,t)}{\partial x}\right] \tag{2}$$

with boundary and initial conditions

$$C(0,t) = C_0,\ C(\infty,t) = 0,\ C(0,0) = C_0,\ C(x>0,0) = 0, \tag{2a}$$

where $C(x,t)$ is the concentration of vaporized material; D_C is the diffusion coefficient of considered material. The concentration dependence of the diffusion coefficient could be written as $D = D_{ass}\{1+\xi\ [C(x,t)/P(x,T)]^{\gamma}\}$ (see, for example, [12]), where $P(x,T)$ is the solubility of the vaporized material. Next, let us to solve Eqs. (1) and (2) by method of averaging of function corrections [13]. Framework this method, we replace the unknown functions $T(x,t)$ and $C(x,t)$ by their unknown average values α_{1T} and α_{1C} in the right-hand sides of the considered equations. Then we obtain the equations for the first-order approximations of the considered functions $T_1(x,t)$ and $C_1(x,t)$

$$c_p\rho\frac{\partial T_1(x,t)}{\partial t} = p(x,t),\ \frac{\partial C_1(x,t)}{\partial t} = 0. \tag{3}$$

Solutions of the above equations could be written as

$$c_p\rho T_1(x,t) = \int_0^t p(x,\tau)\,d\tau + T_r,\ C_1(x,t) = C_0. \tag{4}$$

The second-order approximations of the required functions $T(x,t)$ and $C(x,t)$ have been determined by the framework of standard procedure [13,14], i.e. by replacing these functions by the following sums: $T(x,t)\to\alpha_{2T}+T_1(x,t)$ и $C(x,t)\to\alpha_{2C}+C_1(x,t)$ on the right side of equations (2), where α_{2T} and α_{2C} are the average values of the second-order approximations of the considered temperature $T_2(x,t)$ and concentration $C_2(x,t)$. Higher-order approximations could be calculated similarly with a corresponding increasing of number of order of approximation. The relations for the second-order approximations of the considered functions after the above substitution take the following form

$$c_p\rho\frac{\partial T_2(x,t)}{\partial t} = \lambda_{ass}\frac{\partial}{\partial x}\left(\left\{1+\frac{\mu T_d^{\varphi}}{[\alpha_{2T}+T_1(x,t)]^{\varphi}}\right\}\frac{\partial T_1(x,t)}{\partial x}\right) + c_p\rho u(t)\frac{\partial T_1(x,t)}{\partial x} + p(x,t), \tag{5a}$$

$$\frac{\partial C_2(x,t)}{\partial t} = D_{ass}\frac{\partial}{\partial x}\left\{1+\xi\frac{[\alpha_{2C}+C_1(x,t)]^{\gamma}}{P^{\gamma}(x,T)}\frac{\partial C_1(x,t)}{\partial x}\right\} + u(t)\frac{\partial C_1(x,t)}{\partial x}. \tag{5b}$$

Integration of the left and right sides of equation (5*a*) and (5*b*) on time gives a possibility to obtain the following relations for required approximations of the considered functions

$$c_p\rho T_2(x,t) = \lambda_{ass}\frac{\partial}{\partial x}\int_0^t\left\{1+\frac{\mu T_d^{\varphi}}{[\alpha_{2T}+T_1(x,\tau)]^{\varphi}}\right\}\frac{\partial T_1(x,\tau)}{\partial x}d\tau + c_p\rho\int_0^t u(\tau)\frac{\partial T_1(x,\tau)}{\partial x}d\tau + \int_0^t p(x,\tau)\,d\tau + c_p\rho T_r, \tag{6a}$$

$$C_2(x,t)=D_{ass}\frac{\partial}{\partial x}\int_0^t\left\{1+\xi\frac{[\alpha_{2C}+C_1(x,\tau)]^\gamma}{P^\gamma(x,T)}\frac{\partial C_1(x,\tau)}{\partial x}\right\}d\tau+\int_0^t u(\tau)\frac{\partial C_1(x,\tau)}{\partial x}d\tau+C_0. \quad (6b)$$

Average values of the second-order approximations of considered functions α_{2T} and α_{2C} could be calculated by using the following standard relations [13]

$$\alpha_{2T}=\frac{1}{\Theta L}\int_0^\Theta\int_0^L[T_2(x,t)-T_1(x,t)]\,d\,x\,d\,t,\ \alpha_{2C}=\frac{1}{\Theta L}\int_0^\Theta\int_0^L[C_2(x,t)-C_1(x,t)]\,d\,x\,d\,t. \quad (7)$$

Substitution of relations (4) and (6) into relations (7) gives a possibility to obtain the following results

$$\alpha_{2T}=\frac{1}{\Theta L}\int_0^\Theta(\Theta-t)\int_0^L\left(\frac{\lambda_{ass}}{c_p\rho}\frac{\partial}{\partial x}\left\{1+\frac{\mu T_d^\varphi}{[\alpha_{2T}+T_1(x,t)]^\varphi}\right\}\frac{\partial T_1(x,t)}{\partial x}+\right.$$

$$\left.+c_p\rho u\,(t)\frac{\partial T_1(x,t)}{\partial x}\right)d\,x\,d\,t, \quad (8a)$$

$$\alpha_{2C}=\frac{1}{\Theta L}\int_0^\Theta(\Theta-t)\int_0^L\left(D_{ass}\frac{\partial}{\partial x}\left\{1+\xi\frac{[\alpha_{2C}+C_1(x,t)]^\gamma}{P^\gamma(x,T)}\frac{\partial C_1(x,t)}{\partial x}\right\}+\right.$$

$$\left.+u(t)\frac{\partial C_1(x,t)}{\partial x}\right)d\,x\,d\,t. \quad (8b)$$

The average values of α_{2T} and α_{2C} depend on values of parameters μ and φ. Framework this paper, we calculate concentration of the growth component and temperatures are as the second-order approximations framework the method of averaging functional corrections. The approximations are usually enough adequate approximations for obtaining qualitative consequences and obtaining some quantitative results. The results of analytical calculations were verified by comparison of them with results of numerical simulation.

DISCUSSION

In this section, we have analyzed spatio-temporal distribution of concentration of vaporized material. Figs. 2 and 3 show dependences of concentration of vaporized material of frequency of laser pulses and temperature of substrate at fixed value of other parameter. The increasing of this concentration is natural, because with an increasing of the temperature and frequency of the laser pulses lead to increasing of quantity of evaporated material. Fig. 4 shows dependences of concentration of vaporized material on pressure in growth chamber.

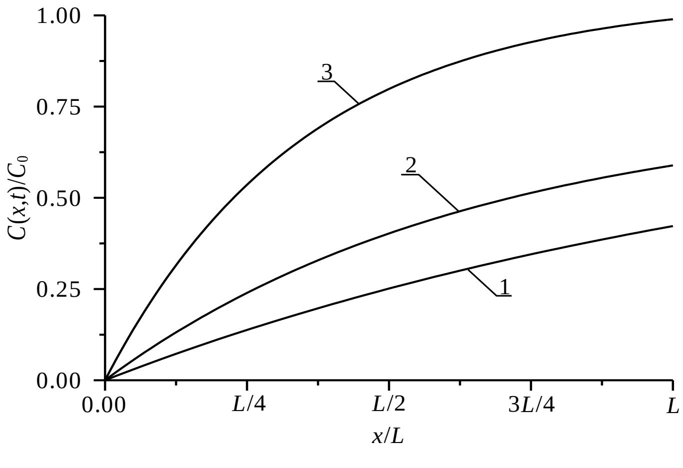

Fig. 2. Distributions of the concentration of the growth component at various values of the laser pulse frequency. Increasing of curve number corresponds to increasing of the laser pulse frequency

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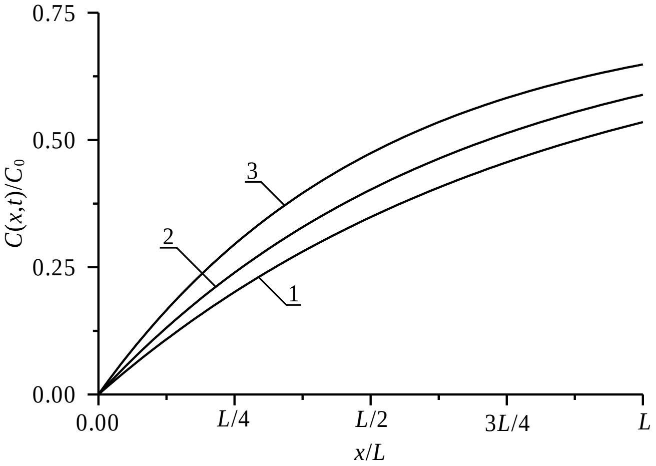

Fig. 3. Distributions of the concentration of the growth component at various values of temperature of the substrate. Increasing of curve number corresponds to increasing of the temperature

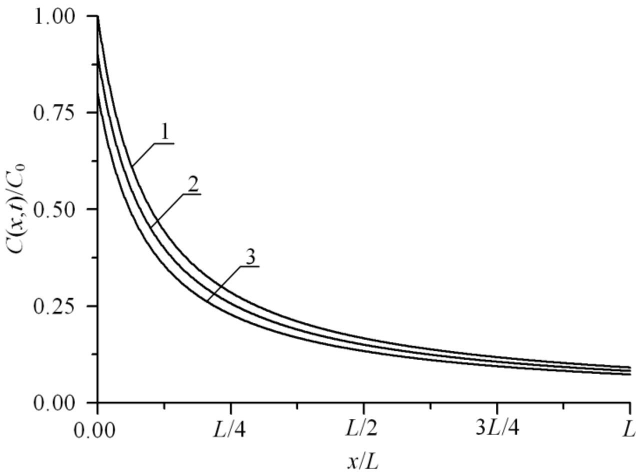

Fig. 4. Distributions of the concentration of the growth component at various values of pressure in growth chamber. Increasing of curve number corresponds to increasing of the pressure

CONCLUSION

We consider an analytical approach for analysis of mass and heat transfer during pulse laser deposition in a reaction chamber during growth of epitaxial layer. The approach gives a possibility to take into account changing of parameters of processes both in space and time, as well as the nonlinearity of the processes (in this situation the approach could be consider as more adequate prognosis in comparison with previously considered approaches). We analyzed changing of mass and heat transfer in the reaction chamber under influence of variation of parameters.

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